

Tatarinoid B

Inchi:	InChI=1S/C12H16O5/c1-7(13)12(14)8-5-10(16-3)11(17-4)6-9(8)15-2/h5-6,12,14H,1-4H3
InchiKey:	LVZSTCWLAWIFNV-UHFFFAOYSA-N
Formula:	C12H16O5
SMILES:	COc1cc(OC)c(C(O)C(C)=O)cc1OC
Mol. weight [g/mol]:	240.25
CAS:	1229005-36-0

Physical Properties

Property code	Value	Unit	Source
gf	-449.50	kJ/mol	Joback Method
hf	-755.64	kJ/mol	Joback Method
hfus	25.44	kJ/mol	Joback Method
hvap	76.83	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.335		Crippen Method
mcvol	181.230	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1847.20		NIST Webbook
tb	728.45	K	Joback Method
tc	925.99	K	Joback Method
tf	451.42	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.35	J/molxK	728.45	Joback Method
cpg	550.77	J/molxK	893.07	Joback Method
cpg	541.77	J/molxK	860.15	Joback Method
cpg	532.02	J/molxK	827.22	Joback Method
cpg	521.51	J/molxK	794.30	Joback Method
cpg	510.28	J/molxK	761.37	Joback Method
cpg	558.98	J/molxK	925.99	Joback Method
dvisc	0.0000233	Paxs	728.45	Joback Method

dvisc	0.0000329	Paxs	682.28	Joback Method
dvisc	0.0000487	Paxs	636.11	Joback Method
dvisc	0.0000767	Paxs	589.93	Joback Method
dvisc	0.0001305	Paxs	543.76	Joback Method
dvisc	0.0002449	Paxs	497.59	Joback Method
dvisc	0.0005228	Paxs	451.42	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1229005360&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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